Simulation of Crystal Extraction Experiments

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Abstract

We discuss the simulation methods and results for the crystal extraction experiments performed recently at the high energy accelerators. Possible future applications of the crystal channeling technique are considered.

1 Introduction

Crystal extraction experiments have greatly progressed in recent years, spanning over two decades in energy and more than two decades in the crystal bending angle[1, 2, 3]. The theory of crystal extraction is essentially based on Monte Carlo simulations, as the extraction process includes multiple passes through the crystal, and turns in the accelerator, of the beam particles. Even more importantly, tracking of a particle through a bent crystal lattice requires not only a calculation of a particle dynamics in this nonlinear field, but also a generation of random events of scattering on the crystal electrons and nuclei.

To track particles through the curved crystal lattices in simulation we apply the approach with a continuous potential introduced by Lindhard. In this approach one considers collisions of the incoming particle with the atomic strings or planes instead of with separate atoms, if the particle is sufficiently aligned with respect to the crystallographic axis or plane. The typical step size along the crystal length in simulation is about 1 micron, as defined by the particle dynamics in crystal channel. By every step the probabilities of scattering events on electrons and nuclei are computed depending on their local densities which are functions of coordinates. This ensures correct orientational dependence of all the processes in crystal material. Further details on the simulation code may be found in Refs.[4, 5].

Leaving aside the details of channeling physics, it may be useful to mention that accelerator physicist will find many familiar things there:

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- Channeled particle oscillates in a transverse nonlinear field of a crystal channel, which is the same thing as the "*betatronic oscillations*" in accelerator, but on a much different scale (the wavelength is 0.1 mm at 1 TeV in silicon crystal). The number of oscillations per crystal length can be several thousand in practice. The concepts of beam emittance, or particle action have analogs in crystal channeling.

- The crystal nuclei arranged in crystallographic planes represent the "*vacuum chamber walls*". Any particle approached the nuclei is rapidly lost from channeling state. Notice a different scale again: the "vacuum chamber" size is $\sim$2 Å.

- The well-channeled particles are confined far from nuclei (from "aperture"). They are lost then only due to scattering on electrons. This is analog to "*scattering on residual gas*". This may result in a gradual increase of the particle amplitude or just a catastrophic loss in a single scattering event.

- Like the real accelerator lattice may suffer from *errors of alignment*, the lattice of real crystal may have dislocations too, causing an extra diffusion of particle amplitude or (more likely) a catastrophic loss.

- Accelerators tend to use low temperature, superconducting magnets. Interestingly, the crystals cooled to *cryogenic temperatures* are more efficient, too.

2 The SPS Experiments

A detailed account for the crystal extraction experiments made at the CERN SPS can be found in this volume[2]. Before these SPS studies, the theoretical comparisons [6] with extraction experiments [7, 8] were restricted by analytical estimates only, which gave the right order of magnitude. The computer simulations considered idealized models only and predicted the extraction efficiencies always in the order of 90–99% (e.g. [6]) while real experiments handled much smaller efficiencies, in the order of 0.01 % [7, 8].

The considered-below theoretical work has been the first and rather detailed comparison between the realistic calculation from the first principles (computer simulation) and the experiment. The simulation was performed [9] with parameters matching those of the SPS experiment. Over 10^5 protons have been tracked both in the crystal and in the accelerator for many subsequent passes and turns until they were lost either at the aperture or in interaction with crystal nuclei.

In the simulation, different assumptions about quality of the crystal surface were applied: one was an ideal surface, whereas the other one assumed near-surface irregularities (a 'septum width') of a few μm due to a miscut angle (between the Si(110) planes and the crystal face) 200 μrad, surface nonflatness 1 μm, plus 1 μm thick amorphous layer superposed. Two options were considered. The *first*, with impact parameter below 1 μm and surface parameters as described above, excludes the possibility of channeling in the first pass through the crystal. This is compared to the *second* option, in which the crystal surface is assumed perfect, i.e., with a zero septum width.

Table 1 shows the expected extraction efficiencies for both options from the

Table 1: SPS crystal extraction efficiencies from the early runs, Monte Carlo and experiment

Option	Monte Carlo	Experiment
Poor surface	15%	lower limit of 2-3%
Ideal surface	40%	only known

first simulation run and the measured lower limit of extraction efficiency as presented at the 19-th meeting on "SPS Crystal Extraction" [10] held at CERN.

Though the efficiency comparison, theory to measurements, was not possible at that time, from the analysis of the simulation results one could see that the perfect-surface simulation predicted narrow high peaks for the angular scans (30 μrad FWHM) and extracted-beam profiles, which have not been observed. The imperfect-surface option, however, is approximately consistent with the experimental observations: wide (about 200 μrad FWHM) angular scan and sophisticated profiles of the extracted beam (dependent on the crystal alignment).

The efficiency was measured in the SPS experiment with that first tested crystal to be 10$\pm$1.7%. The detailed simulations have shown that efficiency should be a function of the vertical coordinate of the beam w.r.t. the crystal (for its given shape), and be from 12 to 18% at peak, with imperfect-surface option.

The simulation studies for a new crystal with another geometry ("U-shaped") were performed prior to the measurements. The model followed the parameters and design of this crystal, with the same SPS setting. Again the two options, an imperfect or perfect edge, have been studied.

Figure 1 shows the angular scan (as narrow as 70 μrad FWHM) of the efficiency simulated for the U-shaped crystal with edge imperfections; a comparison to the measurements shows a good agreement. The peak efficiency, 19.5$\pm$0.7%, was expected to be just slightly increased with the new crystal. For an ideal crystal and a parallel incident beam, the simulation predicted a peak efficiency of $\sim$50% and a very narrow angular scan (25 μrad FWHM).

Another SPS experiment employed a crystal with an amorphous layer at the edge to suppress the channeling in the first passage of the protons [2]. The extraction efficiency with this crystal was indeed of the same order of magnitude as found without an amorphous layer, thus confirming the theoretical prediction [9] that the first-pass channeling is suppressed in the SPS crystals.

In order to understand some overestimate of the peak efficiency in the model, we made a more detailed simulation [11]. Overestimate of the channeling efficiency might mean an underestimate of the scattering and/or losses in the multipasses in crystal. It is clear that the parameters influencing crystal extraction are not defined perfectly; there are several unknowns in the model, such as the impact parameters and quality of the crystal edge.

In the subsequent simulations the realistic details of the crystal design, such

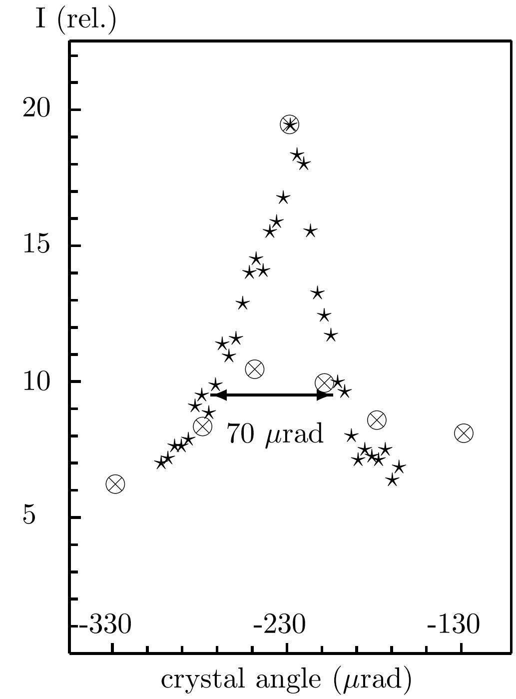

Figure 1: The angular scan of extraction with a U-shaped crystal. Prediction ($\otimes$) and measurement ($\star$).

as the "legs of U" (the scattering here was missed previously) were introduced. The window for the extracted protons was ± 30 μrad (± 2 θ_c) from the extraction line, in order to match the experimental procedure (earlier, all protons bent at >8.0 mrad were accepted).

Table 2 shows the computed peak efficiency as a function of the septum width t (modelled as an amorphous layer) of the U-shaped crystal. The dependence on t is rather weak; this agrees with the experiment where the 30-μm amorphous layer did not affect the efficiency.

These simulations have been repeated with the energies of 14 and 270 GeV, where new measurements have been done at the SPS. The results are shown in Table 3.

Table 2: The peak efficiency F (%) for different septum widths t (μm). The statistical error is 0.6 %.

t (μm)	1	20	50	100	200
F (%)	13.9	12.4	12.9	10.9	8.2

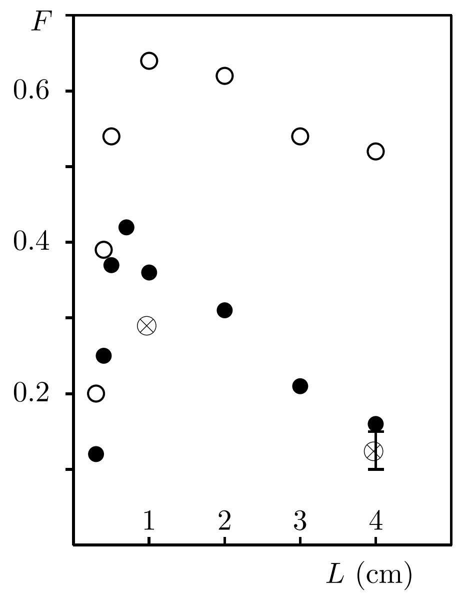

Figure 2: The SPS extraction efficiency vs crystal length. For a perfect surface (o) and septum width t=1 μm ($\bullet$). The $\otimes$ are for the U-shaped design and t=20 μm. Also shown is the measured range of efficiencies, 10–15% for the 4-cm U-shaped crystal.

The length of the Si crystal used in the experiment is optimal to bend the 120 GeV proton beam by 8.5 mrad with a *single* pass. The efficiency of the *multi*-pass extraction is defined by the processes of channeling, scattering, and nuclear interaction in the crystal, which depend essentially on the crystal length L. As the scattering is added, it is qualitatively obvious that the optimal length is reduced as compared to bending with a single pass.

The optimization with the simulations was made with the assumption of a uniform crystal curvature, Fig. 2. For a perfect surface there is almost no dependence for $L \geq 1$ cm in the range studied, but for an imperfect surface there is an important dependence. A new optimum around $L \simeq 0.7$ cm almost doubles the efficiency as compared to that for the 3 cm crystal. Figure 2 shows also two points from a simulation with a U-shaped design and t=20 μm. The shorter crystal had 1-mm "legs" and 8-mm bent part (10 mm in total), and has shown an efficiency near 30 %.

3 The Tevatron Experiment

The Tevatron extraction experiment has provided another check of theory at a substantially higher energy of 900 GeV. A detailed report of predictions for this experiment from the Monte Carlo simulations was published in Ref. [5], and the experimental data can be found in [3].

In our computer model we have investigated three options: a crystal with ideal surface, one with a septum width (amorphous layer) of t=1 μm, and one with t=50 μm. The crystal bending shape and other details were as used later in the experiment. Figure 3 from Ref.pre3 shows that there is little difference between the three options; the peak efficiency is about 35-40%, and the angular

scan FWHM is 50-55 μrad. This insensitivity to the crystal surface quality is due to the set-up different from that used in other experiments; as a result, the starting divergence of incident protons at the crystal was not small and hence less sensitive to edge scattering.

The measured peak efficiency was about 30%. This value, together with the measured angular scan, is superimposed in Figure 3 on the theoretical expectation, showing a rather good agreement.

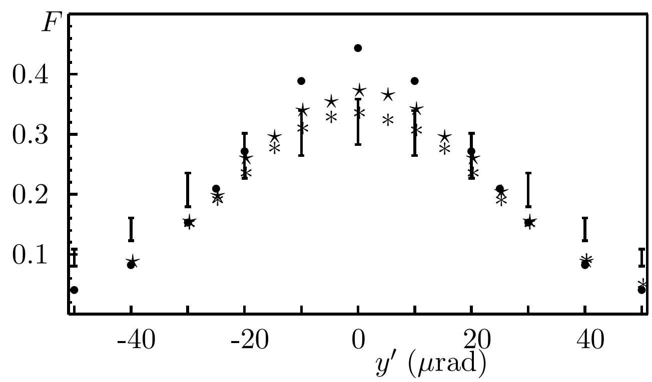

Figure 3: Vertical angular scan of the overall efficiency for the perfect horizontal alignment, x'=0. Ideal crystal ($\bullet$); imperfect crystal: ($\star$) with t=1 μm, ($*$) is the same with t=50 μm. Also shown is the measured peak efficiency and angular scan.

The efficiency of extraction can again be increased with the use of a shorter crystal. Fig. 4 shows the extraction efficiency dependence on the crystal length L, for uniform bending of crystal. The efficiency is maximal, near 70 %, in the length range from 0.4 to 1.0 cm.

4 Analytical Theory of Multipass Crystal Extraction

An analytical theory of multipass crystal extraction would be highly helpful in understanding the experimental results. Below we describe a simple theory for the extraction efficiency [12].

Suppose that a beam with divergence σ, Gaussian distribution, is aligned to the crystal planes. Then as many as

$$(2\theta_c/\sqrt{2\pi}\sigma)(\pi x_c/2d_p) \tag{1}$$

particles get channeled in the initial straight part of the crystal. Here θ_c stands for the critical angle of channeling, d_p the interplanar spacing, $x_c \approx d_p/2 - a_{TF}$ the critical distance, a_{TF} being the Thomas-Fermi screening distance.

We shall first consider the case where particles first come to the crystal with nearly zero divergence, due to very small impact parameters. We assume then that any particle always crosses the full crystal length; that pass 1 is like through an amorphous matter but any further pass is like through a crystalline matter; that there are no aperture restrictions; and that the particles interact only with

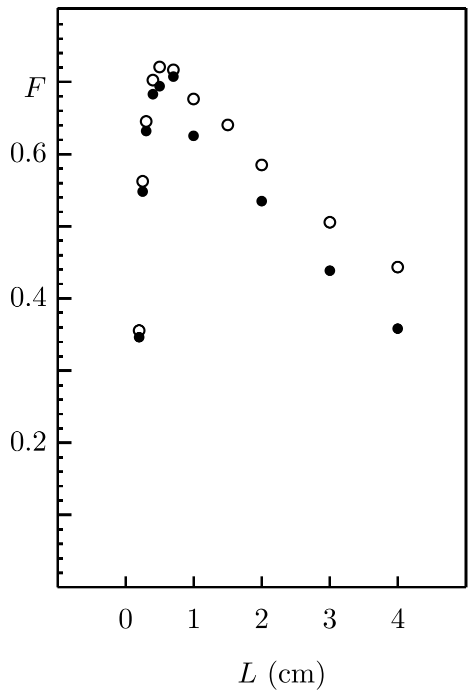

Figure 4: Efficiency as a function of L for the ideal (o) and imperfect (•), t=1 μm, crystals.

the crystal not a holder. After some turns in the accelerator ring, the scattered particles come to the crystal with rms divergence as defined by scattering in the first pass:

$$\sigma_1 = (E_s/pv)(L/L_R)^{1/2}, \tag{2}$$

where E_s=13.6 MeV, L is the crystal length, L_R the radiation length, pv the particle momentum times velocity.

After k passes the divergence is $\sigma_k = k^{1/2}\sigma_1$. The number of particles lost in nuclear interactions is $1-\exp(-kL/L_N)$ after k passes; L_N is the interaction length. In what follows we shall first assume that the crystal extraction efficiency is substantially smaller than 100 % (which has actually been the case so far), i.e. the circulating particles are removed from the ring predominantly through the nuclear interactions, not through channeling.

That pulled together, we obtain the multipass channeling efficiency by summation over k passes, from 1 to infinity:

$$F_C = \left(\frac{\pi}{2}\right)^{1/2} \frac{\theta_c x_c}{\sigma_1 d_p} \times \Sigma(L/L_N) \tag{3}$$

where

$$\Sigma(L/L_N) = \Sigma_{k=1}^{\infty} k^{-1/2} \exp(-kL/L_N) \tag{4}$$

may be called a "multiplicity factor" as it just tells how much the single-pass efficiency is amplified in multipasses.

A fraction $1-T$ of channeled particles is to be lost along the bent crystal due to scattering processes and centripetal effects. Then the multipass extraction efficiency is

$$F_E = F_C \times T = \left(\frac{\pi}{2}\right)^{1/2} \frac{\theta_c x_c}{\sigma_1 d_p} \times \Sigma(L/L_N) \times T \tag{5}$$

We shall use an analytical approximation (as used also in [13]) for silicon

$$T = (1-p/3R)^2 \exp\left(-\frac{L}{L_d(1-p/3R)^2}\right), \tag{6}$$

where p is in GeV/c, and R is in cm; L_d is dechanneling length for a straight crystal. The first factor in T describes a centripetal dechanneling. E.g., at pv/R=0.75 GeV/cm (which is close to the highest values used in extraction) our approximation gives $(1-p/3R)^2$=0.563 whereas Forster et al.[14] measured 0.568±0.027. We shall use the theoretical formula for L_d [11]. The sum (4) can be approximated as follows:

$$\Sigma(L/L_N) \simeq (\pi L_N/L)^{1/2} - 1.5 \tag{7}$$

Let us check the theory, first against the CERN SPS data [15] where the crystal extraction efficiency was measured at 14, 120, and 270 GeV (Table 1).

Table 3: Extraction efficiencies (%) from the SPS experiment, theory, and detailed simulations.

pv(GeV)	SPS	Theory	Monte Carlo
14	0.55±0.30	0.30	0.35±0.07
120	15.1±1.2	13.5	13.9±0.6
270	18.6±2.7	17.6	17.8±0.6

The Tevatron extraction experiment at 900 GeV provides another check. Here a slight modification of the formulas is needed to account for the non-zero starting divergence, namely σ_0=11.5 μrad (rms). This results in the change in Eq.(4):

$$\Sigma(L/L_N) = \Sigma_{k=1}^{\infty}(k+\sigma_0^2/\sigma_1^2)^{-1/2}\exp(-kL/L_N) \tag{8}$$

Since in this experiment Si(111) planes were used, consisting of narrow (1/4 weight) and wide (3/4 weight) channels, this is to be taken into account in Eq.(5). Eq.(5) then gives an extraction efficiency of 40.8 %. However, a minor correction to the theoretical value is discussed below.

As the extraction efficiency is getting high, our earlier assumption that the nuclear interactions dominate over the crystal channeling may need correction. To take into account the fact that the circulating particles are efficiently removed from the ring by a crystal extraction as well, one would require a *recurrent* procedure of summation: instead of ΣF_k one has to sum ΣF_k^*, where F_k^*=$F_k(1-F_{k-1}^*)$. This “recurrent” correction doesn’t affect our earlier SPS calculation at 14 GeV and makes ~1% drop to the efficiencies at 120 and 270 GeV listed in Table 1. For

Tevatron this correction constitutes −6.7%, converting 40.8% into 34.1%, more into line with the measurement.

To see the dependence of extraction efficiency on the microscopic properties of the crystal material and on the particle energy, let us use the well-known theoretical expressions for θ_c=$(4\pi N d_p Z e^2 a_{TF}/pv)^{1/2}$, radiation length L_R=$137/[4Z(Z+1)r_e^2 N \ln(183Z^{-1/3})]$, and E_s=$2\sqrt{2\times137}m_e c^2$, where N is the number of atoms per unit volume of crystal. The multipass extraction efficiency is then

$$F_E = \frac{\pi}{4}\left(\frac{x_c^2 a_{TF}}{L(Z+1)d_p r_e \ln(183Z^{-1/3})}\right)^{1/2} \times \left(\frac{pv}{m_e c^2}\right)^{1/2} T\Sigma(L/L_N) \tag{9}$$

here m_e is the electron mass, r_e the classical electron radius. Despite of the simplifications done, this equation still predicts the SPS efficiency of 15.7% at 120 GeV which is within the experimental error limits.

Figure 5 shows the $F_E(L)$ dependence for extraction at the 120-GeV SPS, 900-GeV Tevatron, and 7-TeV Large Hadron Collider (where 0.7 mrad deflection angle is assumed); in all the cases the crystal bent part was 0.75 of the full length. One can see that the analytical dependences $F_E(L)$ are very close to those obtained earlier in Monte Carlo simulations [16]. The same maxima at the same optimal lengths are predicted.

Formula (5) predicts a high efficiency of multipass extraction at a multi-TeV LHC, about 45 %, with the optimal length of Si(110) crystal being 6±1 cm.

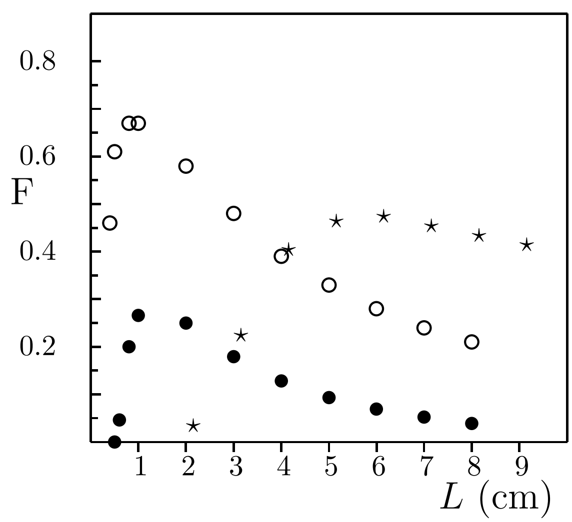

Figure 5: The extraction efficiency, Eq.(5), as a function of the crystal length L; for the SPS (•), Tevatron (o), and Large Hadron Collider ($\star$).

5 IHEP Experiment

The pioneering crystal extraction experiments at Protvino IHEP 70-GeV accelerator were made [8] before any computer simulations of this kind. This is why

we prefer to mention a new IHEP experiment planned for November 1997 where one could make predictions in advance.

This experiment employs a very short (7 mm along the beam) silicon crystal bent a small angle of 1.75 mrad. Figure 6 shows the angular scan of the extraction efficiency as seen in Monte Carlo simulations. The peak efficiency is rather modest, about 20%, because of a big effective divergence of the protons at crystal w.r.t. the crystal planes (part of it is due to the crystal design, another part is due to the beam phase space geometry).

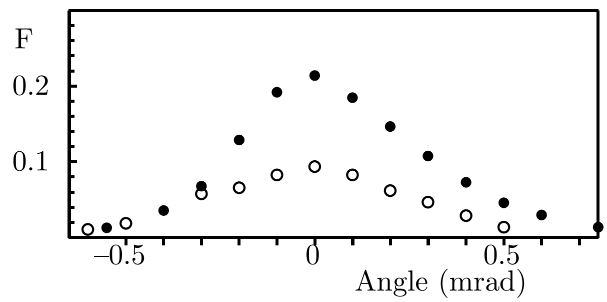

Figure 6: The angular scan of the extraction efficiency as seen in Monte Carlo simulations for 70-GeV IHEP experiment. Crystal without targets (•), and with Be target (o).

As the experiment would also investigate a co-existence of crystal extraction with simultaneous work of two internal targets, this option was simulated as well. We have seen practically no influence on the crystal efficiency from a very thin carbon target, whereas a 3-cm long beryllium target could decrease the extraction efficiency (defined as the ratio of protons extracted to protons lost in nuclear interactions in the crystal) up to factor of two. Figure 6 shows the angular scan in this case also.

6 Future Applications

The progress in crystal extraction studies at CERN and Fermilab has been stimulated by the prospects of application of this technique for extraction of a parasitic beam from a large hadron collider for a fixed target physics. Such an extraction is quite feasible from the standpoint of channeling physics. The theory and simulations predict the extraction efficiency of about 50% even under the most conservative assumptions on the crystal design and edge quality.

Another discussed option is extraction from the Tevatron [13] with required minimal angle of 16.4 mrad. In our simulations of this option with use of the same set-up as in the E853 experiment, the efficiency is expected to be 6.3±0.7% with Si crystal of ∼12 cm length even if the first-pass channeling is fully suppressed. However, if channeling in the first encounter is efficient (good crystal edge), the efficiency becomes as high as 23% with the use of optimal 5-cm long Ge(110) crystal. Notice, that this figure—over 20% efficiency of bending at 16.4 mrad by a Ge(110) crystal—is already demonstrated experimentally at CERN with a 200 GeV beam [17]!

One very interesting option is a crystal use in the beam collimation systems. A principle problem for an amorphous collimator is the edge scattering causing a leak of particles incident closer than $\sim$1 μm to the collimator edge. Furthermore, if collimator of length L is misaligned by an angle θ, the inefficient edge thickness is increased by $L\theta$; therefore, an amorphous collimator should be aligned with accuracy of order $\theta \ll 1$ μm$/L \simeq 2$ μrad (for L=450 mm[18])! Compare this with critical angles for crystals—order of 20 μrad at 100 GeV and order of 2 μrad at 7 TeV. Of course, it is much easier to align crystals than huge collimators.

An edge leak doesn't exist in crystalline material for channeled particles. The simplest idea is to put a bent crystal in front and at the edge of a heavy collimator. A large fraction of incident particles is bent by the crystal some small angle of 0.1-0.3 mrad toward the depth of the collimator, and hence fully absorbed (this idea has something common with the idea of a magnetized collimator[18]). The collimator has only to deal with the remaining particles, unchanneled in crystal. According to our Monte Carlo simulations, the efficiency of bending of a parallel beam is about 90% for a 1-TeV beam and 2-cm long Si(110) crystal bent 0.2 mrad, and for a 7-TeV beam and 5-cm long Si(110) crystal bent 0.1 mrad. Notice, that the experimentally demonstrated record of bending efficiency at CERN is already 60% for 2 mrad bending angle at the energy of 0.45 TeV [17]! Hence, under the optimal conditions the inefficiency the collimation system can be reduced by factor of 10. If it were a two-stage collimation system, and both stages equipped by bent crystals, the inefficiency of the whole system would be reduced by factor of 100.

Notice that this simplest idea doesn't affect the optics of the collimation design. One could take the existing collimation system and just add crystals to improve its efficiency.

More advanced idea would be to separate a bent crystal from a heavy collimator, and to optimize its position w.r.t. the collimator. This idea has been discussed and simulated in Ref.[19].

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